Emilio L Angelina

List of Publications by Year
in descending order

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21	363	933447 10	794594 19
papers	citations	h-index	g-index

21	21	21	407
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular Modeling Study of Dihydrofolate Reductase Inhibitors. Molecular Dynamics Simulations, Quantum Mechanical Calculations, and Experimental Corroboration. Journal of Chemical Information and Modeling, 2013, 53, 2018-2032.	5.4	56
2	Searching the â€œBiologically Relevantâ€Conformation of Dopamine: A Computational Approach. Journal of Chemical Information and Modeling, 2012, 52, 99-112.	5.4	48
3	2,3,9- and 2,3,11-Trisubstituted tetrahydroprotoberberines as D2 dopaminergic ligands. European Journal of Medicinal Chemistry, 2013, 68, 150-166.	5.5	37
4	An integrative study to identify novel scaffolds for sphingosine kinase 1 inhibitors. European Journal of Medicinal Chemistry, 2017, 139, 461-481.	5.5	33
5	Non-covalent interactions in receptor-ligand complexes. A study based on the electron charge density. Journal of Physical Organic Chemistry, 2014, 27, 128-134.	1.9	29
6	On the strength of the halogen bonds: Mutual penetration, atomic quadrupole moment and Laplacian distribution of the charge density analyses. Computational and Theoretical Chemistry, 2012, 998, 164-172.	2.5	24
7	Halogen bonding in biological context: a computational study of D2 dopamine receptor. Journal of Physical Organic Chemistry, 2016, 29, 645-655.	1.9	21
8	New small-size peptides modulators of the exosite of BACE1 obtained from a structure-based design. Journal of Biomolecular Structure and Dynamics, 2017, 35, 413-426.	3.5	17
9	The electronic density obtained from a QTAIM analysis used as molecular descriptor. A study performed in a new series of DHFR inhibitors. Journal of Molecular Structure, 2017, 1134, 464-474.	3.6	16
10	Combining Charge Density Analysis with Machine Learning Tools To Investigate the Cruzain Inhibition Mechanism. ACS Omega, 2019, 4, 19582-19594.	3.5	13
11	Pentameric models as alternative molecular targets for the design of new antiaggregant agents. Current Protein and Peptide Science, 2016, 17, 156-168.	1.4	12
12	3â€Chlorotyramine Acting as Ligand of the D₂ Dopamine Receptor. Molecular Modeling, Synthesis and D₂ Receptor Affinity. Molecular Informatics, 2015, 34, 28-43.	2.5	10
13	Tetrahydroisoquinolines functionalized with carbamates as selective ligands of D2 dopamine receptor. Journal of Molecular Modeling, 2017, 23, 273.	1.8	9
14	Searching new structural scaffolds for BRAF inhibitors. An integrative study using theoretical and experimental techniques. Bioorganic Chemistry, 2019, 91, 103125.	4.1	9
15	Conformational and electronic study of dopamine interacting with the <scp>D₂</scp> dopamine receptor. Journal of Computational Chemistry, 2020, 41, 1898-1911.	3.3	9
16	Hydroxynaphthalenecarboxamides and substituted piperazinylpropandiols, two new series of BRAF inhibitors. A theoretical and experimental study. Bioorganic Chemistry, 2020, 103, 104145.	4.1	8
17	Design, synthesis, biological evaluation and molecular modelling of substituted pyrrolo[2,1-a]isoquinolinone derivatives: discovery of potent inhibitors of AChE and BChE. New Journal of Chemistry, 2021, 45, 8321-8334.	2.8	3
18	Study of polyphenols from Caesalpinia paraguariensis as Î±-glucosidase inhibitors: kinetics and structureâ€“activity relationship. New Journal of Chemistry, 0, , .	2.8	3

#	Article	IF	Citations
19	Flap-site Fragment Restores Back Wild-type Behaviour in Resistant Form of HIV Protease. Molecular Informatics, 2018, 37, 1800053.	2.5	2
20	Covalence and Ï€-electron delocalization influence on hydrogen bonds in proton transfer process of o-hydroxy aryl Schiff bases: A combined NMR and QTAIM analysis. Journal of Chemical Physics, 2021, 155, 054307.	3.0	2
21	Evaluating the conformational space of the active site of <scp>D₂</scp> dopamine receptor. Scope and limitations of the standard docking methods. Journal of Computational Chemistry, 2022, 43, 1298-1312.	3.3	2